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Comparative Analysis of Particle Swarm and Differential Evolution via Tuning on Ultrasmall Titanium Oxide Nanoclusters[1] ERIC INCLAN, Georgia Inst of Tech, JACK LASSESTER, Middle Tennessee State University, DAVID GEOHEGAN, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Optimization algorithms (OA) coupled with numerical methods enable researchers to identify and study (meta) stable nanoclusters without the control restrictions of empirical methods. An algorithm's performance is governed by two factors: (1) its compatibility with an objective function, (2) the dimension of a design space, which increases with cluster size. Although researchers often tune an algorithm's user-defined parameters (UDP), tuning is not guaranteed to improve performance. In this research, Particle Swarm (PSO) and Differential Evolution (DE), are compared by tuning their UDP in a multi-objective optimization environment (MOE). Combined with a Kolmogorov Smirnov test for statistical significance, the MOE enables the study of the Pareto Front (PF), made of the UDP settings that trade-off between best performance in energy minimization ("effectiveness") based on force-field potential energy, and best convergence rate ("efficiency"). By studying the PF, this research finds that UDP values frequently suggested in the literature do not provide best effectiveness for these methods. Additionally, monotonic convergence is found to significantly improve efficiency without sacrificing effectiveness for very small systems, suggesting better compatibility.

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